Inosine

58-63-9 | DTXSID2045993

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 293 °C

Global applicability domain: Outside

Local applicability domain index: 8.87e-02

Confidence level: 4.13e-01

Nearest Neighbors from the Training Set

Image not found
Triisopropanolamine
Measured: 305
Predicted: 302

Image not found
Triethanolamine
Measured: 335
Predicted: 326

Image not found
2,2'-[(4-Methylphenyl)imino]diethanol
Measured: 339
Predicted: 310

Image not found
Metaraminol
Measured: 218
Predicted: 257

Image not found
Flurprimidol
Measured: 264
Predicted: 304